A LINE LIST FOR HYDROGEN SULFIDE

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$H_2S$ is being studied as part of the ExoMol project (www.exomol.com) with the aim of producing an accurate and comprehensive list of line positions and intensitiesfor temperatures up to 2000 K. This will provide an important resource for atmospheric modelling of extrasolar planets and cool stars, as well as for the laboratory investigations and pollution studies. A recently computed, variational ro-vibrational hot line list is presented. These computations used the DVR3D[a] and potential energy surface (PES) refined to reproduce the measured data. An *ab initio* dipole moment surface (DMS) is used for the transitions intensity calculations. Many dipole moment surfaces were constructed at different levels of theory and basis sets, and compared to the available intensity measurements. Our best surface was constructed at over 7000 geometries using CCSD(T)/aug-cc-pV(6+d)Z level of theory with added relativistic and core-electron corrections. The anomalous behavior of $H_2S$ intensities is well-known[b], and our calculations reproduce this behaviour quantitatively. O

With Martin-Drumel and Pirali, we have measured pure rotational transition frequencies of $H_2S$ at room temperature[c] in the 45 to 360 $cm^{-1}$ (1.4 to 10.5 THz) region using a Fourier transform spectrometer located at the AILES beamline of the SOLEIL synchrotron. About 1700 lines were detected belonging to the ground vibrational state of $H_2{}^{32}S$, $H_2{}^{33}S$ and $H_2{}^{34}S$. 60% of these lines are recorded and assigned for the first time, sampling levels as high as $J = 26$ and $K_a = 18$. Our variational calculations were used to identify 214 rotational lines of $H_2{}^{32}S$ in its first excited bending vibrational state for the first time.

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[b] T. Cours, P. Rosmus, and V. G. Tyuterev *J. Chem. Phys.* **117**(223), 2002.
[c] A. A. A. Azzam, S. N. Yurchenko, J. Tennyson, M. Martin-Drumel and O. Pirali *J. Quant.e Spectrosc. Radiat. Transf. (submitted)* 2013.